

## SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name:

Art Unit:

Mail Box and Bldg/Rm Location:

4E-12

Katsay Hbk

Examiner #:

78271 Date: Mar. 19, 2003

Phone Number 308-4717

Serial Number: 09/980,593

Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

MEJ

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

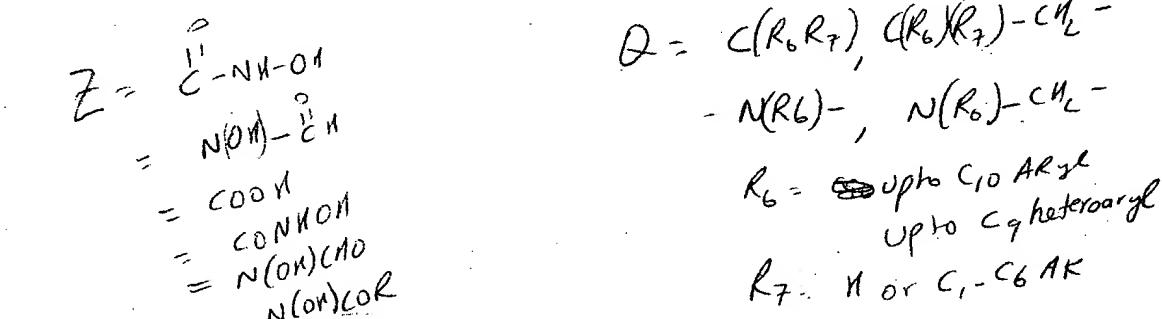
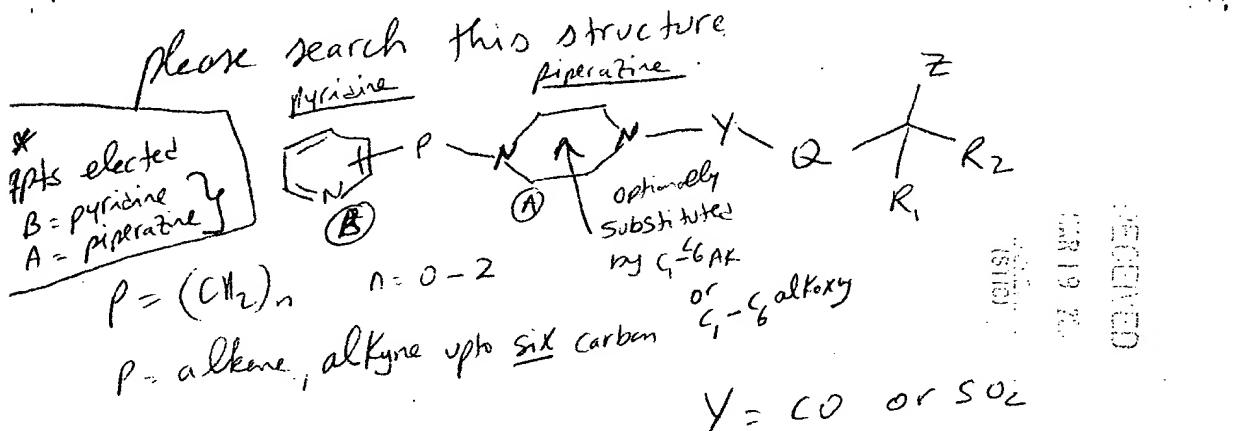
Title of Invention:

Inventors (please provide full names):

Earliest Priority Filing Date: 5/31/2000

\* Please see attached

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.



## STAFF USE ONLY

Searcher: *S. Katsay*Searcher Phone #: *308-47199*

Searcher Location: \_\_\_\_\_

Date Searcher Picked Up: *3/20/03*Date Completed: *3/20/03*

Searcher Prep &amp; Review Time: \_\_\_\_\_

Clerical Prep Time: \_\_\_\_\_

Online Time: \_\_\_\_\_

## Type of Search

NA Sequence (#)

Vendors and cost where applicable

STN

AA Sequence (#)

Dialog

Structure (#)

Questel/Orbit

Bibliographic

Dr. Link

Litigation

Lexis/Nexis

Fulltext

Sequence Systems

Patent Family

WWW/Internet

Other

Other (specify)

=> fil hcaplus  
FILE 'HCAPLUS' ENTERED AT 10:23:53 ON 20 MAR 2003  
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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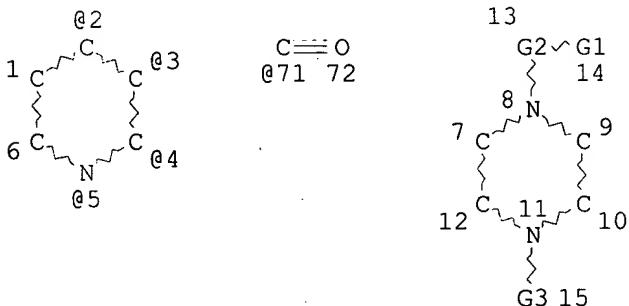
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FILE COVERS 1907 - 20 Mar 2003 VOL 138 ISS 12  
FILE LAST UPDATED: 19 Mar 2003 (20030319/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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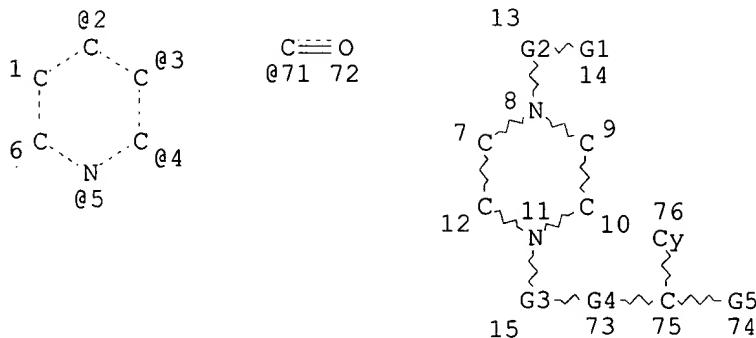
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE  
L5 11004 SEA FILE=REGISTRY SSS FUL L3  
L14 STR



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VAR G1=2/3/4/5
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VAR G4=C/N
VAR G5=71/N
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NUMBER OF NODES IS 21

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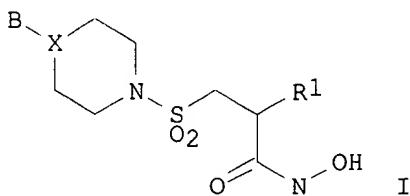
L16 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:636067 HCAPLUS
DOCUMENT NUMBER: 135:195577
TITLE: Preparation of arylpiperazines and arylpiperidines as
       metalloproteinase inhibiting agents
INVENTOR(S): Barlaam, Bernard Christophe; Dowell, Robert Ian;
              Newcombe, Nicholas John; Tucker, Howard; Waterson,
              David
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited
SOURCE: PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

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PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001062751	A1	20010830	WO 2001-GB616	20010215
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
 EP 1261595 A1 20021204 EP 2001-905883 20010215  
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 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
 NO 2002003951 A 20020820 NO 2002-3951 20020820  
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 WO 2001-GB616 W 20010215

OTHER SOURCE(S) : MARPAT 135:195577  
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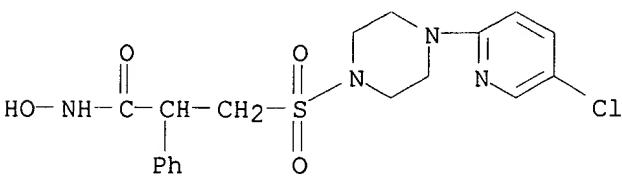
AB The title compds. [I; B = (un)substituted Ph, 2-pyridyl, 2-pyridyloxy, 4-pyrimidinyl; X = C, N; R1 = (trimethyl-1-hydantoin)alkyl, (un)substituted Ph, phenylalkyl, etc.], useful as metalloproteinase inhibitors, esp. as inhibitors of MMP 13, were prepd. E.g., a 5-step synthesis of I [B = 4-FC6H4; X = CH; R1 = CH2Ph] was given.

IT 357187-74-7P 357187-78-1P 357187-79-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of arylpiperazines and arylpiperidines as metalloproteinase inhibiting agents)

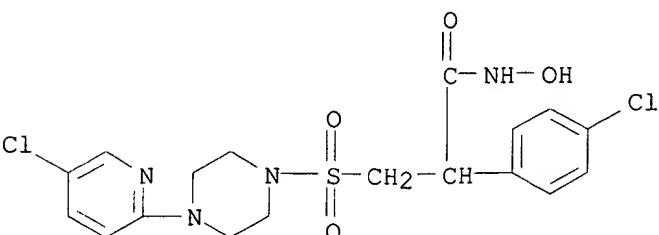
RN 357187-74-7 HCPLUS

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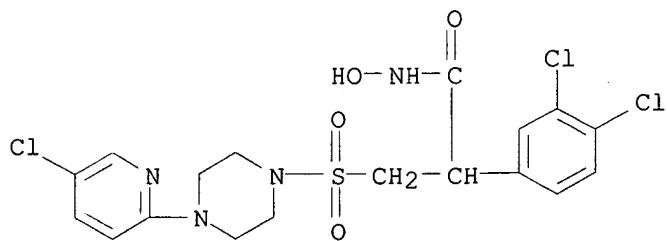


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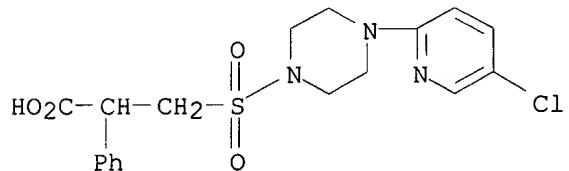


RN 357187-79-2 HCPLUS  
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IT 357187-91-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. of arylpiperazines and arylpiperidines as metalloproteinase inhibiting agents)

RN 357187-91-8 HCPLUS  
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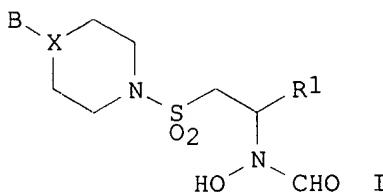


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=&gt;'d ibib abs hitstr 116 2

L16 ANSWER 2 OF 8 HCPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 2001:636059 HCPLUS  
 DOCUMENT NUMBER: 135:211053  
 TITLE: Preparation of N-[2-(piperidino- or piperazino)sulfonylethyl]-N-hydroxyformamides as inhibitors of metalloproteinases  
 INVENTOR(S): Barlaam, Bernard Christophe; Dowell, Robert Ian; Finlay, Maurice Raymond Verschoyle; Newcombe, Nicholas John; Tucker, Howard; Waterson, David  
 PATENT ASSIGNEE(S): AstraZeneca AB, Swed.; AstraZeneca UK Limited  
 SOURCE: PCT Int. Appl., 69 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001062742	A1	20010830	WO 2001-GB624	20010215
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1261590	A1	20021204	EP 2001-905885	20010215
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2002022628	A1	20020221	US 2001-788687	20010221
NO 2002003956	A	20021007	NO 2002-3956	20020820
PRIORITY APPLN. INFO.:			EP 2000-400467 A	20000221
			WO 2001-GB624 W	20010215
OTHER SOURCE(S): GI		MARPAT 135:211053		



AB The title compds. [I; B = (un)substituted Ph, 2-pyridyl, 2-pyridyloxy, 4-pyrimidinyl; X = CH, N; R1 = phenylalkyl, pyridylalkyl, pyrimidinylalkyl, etc.], useful as metalloproteinase inhibitors, esp. as inhibitors of MMP 13 (no data given), were prep'd. E.g., a 4-step synthesis of I [B = 4-BrC6H4; X = N; R1 = 3-(pyrimidin-2-yl)propyl] was given. The compds. I are effective at 0.5-30 mg/kg/day.

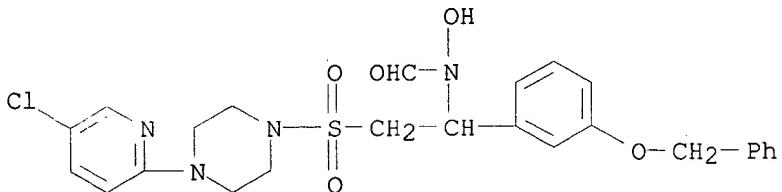
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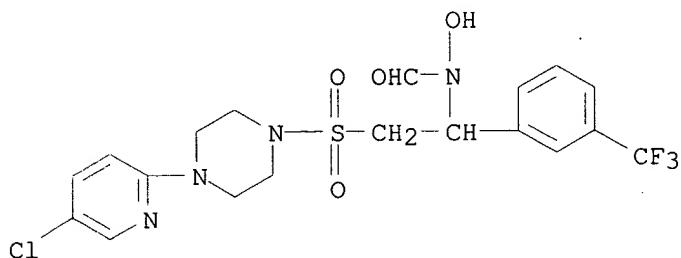
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of N-[2-(piperidino- or piperazino)sulfonylethyl]-N-hydroxyformamides as inhibitors of metalloproteinases)

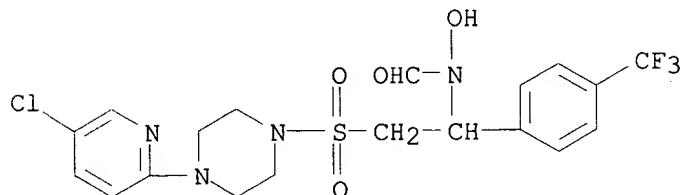
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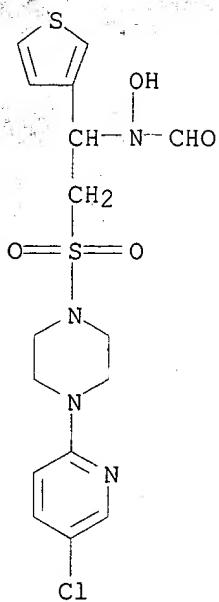
RN 357645-55-7 HCPLUS  
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RN 357645-57-9 HCPLUS  
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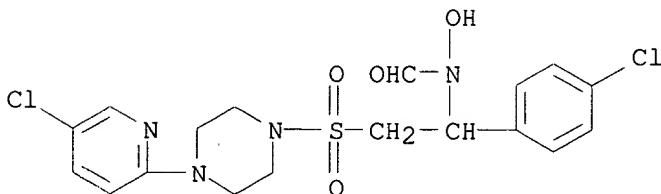


RN 357645-58-0 HCPLUS  
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RN 357646-20-9 HCPLUS

CN Piperazine, 1-[(2-(4-chlorophenyl)-2-(formylhydroxyamino)ethyl)sulfonyl]-4-(5-chloro-2-pyridinyl)- (9CI) (CA INDEX NAME)



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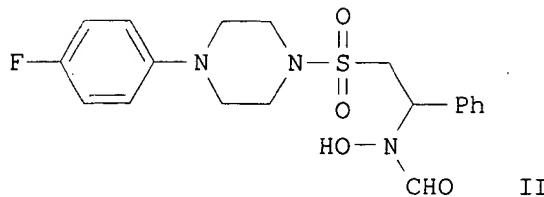
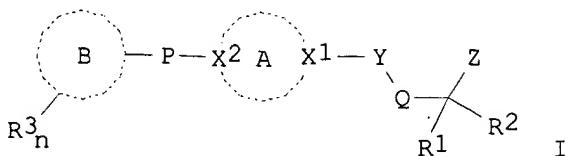
THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L16 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 2000:161258 HCAPLUS  
 DOCUMENT NUMBER: 132:207849  
 TITLE: Preparation of arylpiperazines as metalloproteinase inhibiting agents (MMP)  
 INVENTOR(S): Barlaam, Bernard Christophe; Newcombe, Nicholas John;  
 Tucker, Howard; Waterson, David  
 PATENT ASSIGNEE(S): Zeneca Limited, UK; Zeneca-Pharma Sa  
 SOURCE: PCT Int. Appl., 82 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000012478	A1	20000309	WO 1999-GB2801	19990825
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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AU 9955247	A1	20000321	AU 1999-55247	19990825
BR 9913255	A	20010522	BR 1999-13255	19990825
EP 1109787	A1	20010627	EP 1999-941751	19990825
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EE 200100106	A	20020617	EE 2001-2001001061	19990825
JP 2002523493	T2	20020730	JP 2000-567511	19990825
NO 2001001023	A	20010425	NO 2001-1023	20010228
PRIORITY APPLN. INFO.:			EP 1998-402144	A 19980831
			EP 1999-401351	A 19990604
			WO 1999-GB2801	W 19990825

OTHER SOURCE(S): MARPAT 132:207849  
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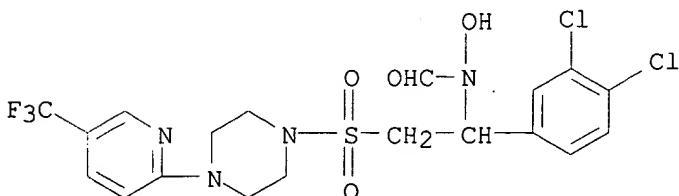
AB The title compds. [I; B = monocyclic or bicyclic alkyl, aryl, etc.; R3 = H, halo, NO<sub>2</sub>, etc.; n = 1-3; P = (CH<sub>2</sub>)<sub>n</sub> (wherein n = 0-2), alkene, alkyne, etc.; A = (un)substituted 5-7 membered aliph. ring; X<sub>1</sub>, X<sub>2</sub> = N, C, where a ring substituent on ring A is a oxo group that is preferably adjacent a ring N atom; Y = SO<sub>2</sub>, CO; Z = CONHOH, Y = CO and Q = CR<sub>6</sub>R<sub>7</sub>, CR<sub>6</sub>R<sub>7</sub>CH<sub>2</sub>, NR<sub>6</sub>, NR<sub>6</sub>CH<sub>2</sub> (wherein R<sub>6</sub> = H, alkyl, aralkyl, etc.; R<sub>7</sub> = H, alkyl; R<sub>7</sub> together with R<sub>6</sub> forms a carbocyclic or heterocyclic spiro 5-7 membered ring, the latter contg. at least one heteroatom selected from N, O, S); Z = CONHOH, Y = SO<sub>2</sub> and Q = CR<sub>6</sub>R<sub>7</sub>, CR<sub>6</sub>R<sub>7</sub>CH<sub>2</sub>; Z = N(OH)CHO and Q = CHR<sub>6</sub>, CHR<sub>6</sub>CH<sub>2</sub>, NR<sub>6</sub>CH<sub>2</sub>; R<sub>1</sub> = H, alkyl, cycloalkyl, etc.; R<sub>2</sub> = H, alkyl, aryl, etc.], useful as metalloproteinase inhibitors (no data), esp. as inhibitors of MMP 13, in treating arthritis and atherosclerosis, were prep'd. E.g., a multi-step synthesis of the title piperazine II was given. Compds. I are effective at 0.5-30 mg/kg/day.

IT  
 260438-29-7P 260438-30-0P 260438-32-2P  
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of arylpiperazines as metalloproteinase inhibiting agents (MMP))

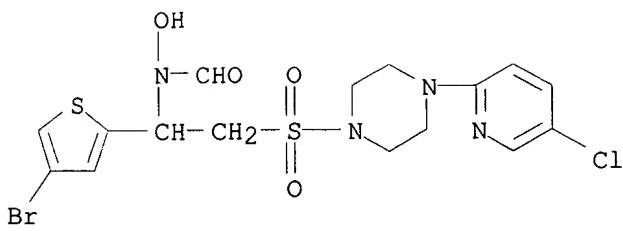
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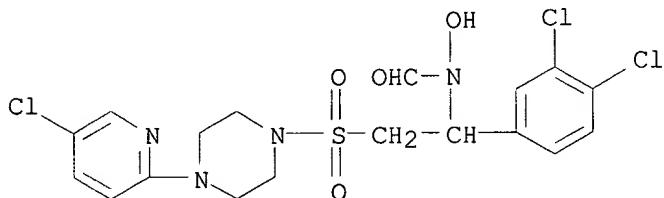


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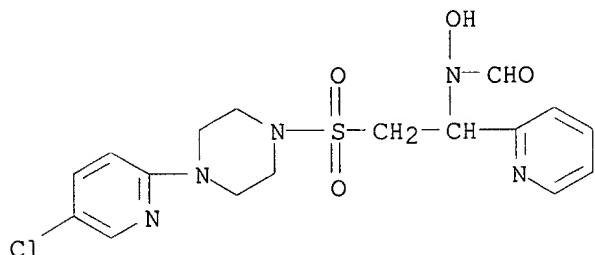
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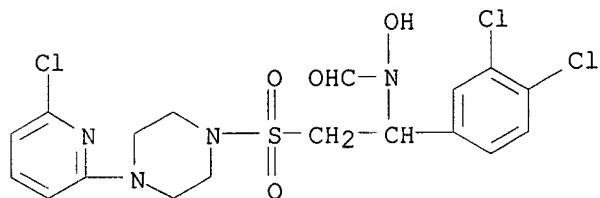
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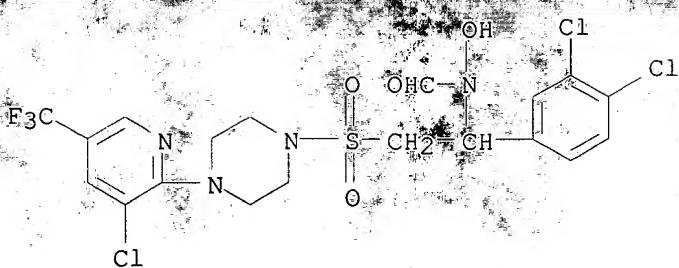
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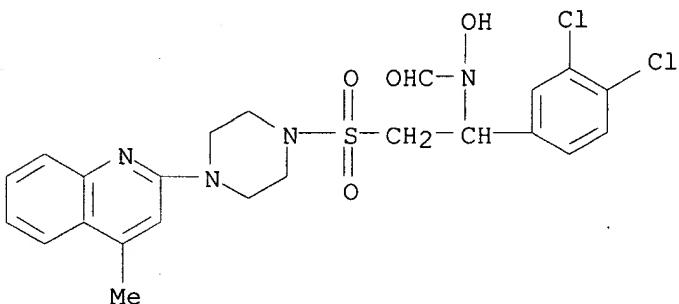


RN 260439-10-9 HCPLUS  
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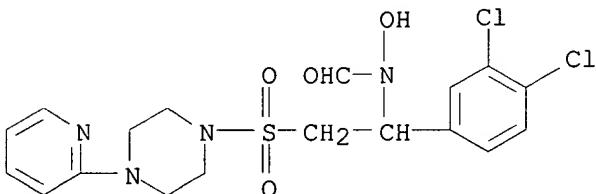
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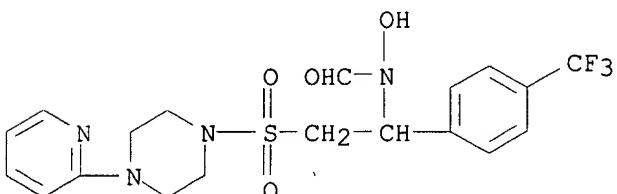
RN 260439-17-6 HCPLUS

CN Piperazine, 1-[(2-(3,4-dichlorophenyl)-2-(formylhydroxyamino)ethyl]sulfonyl-1-4-(2-pyridinyl)- (9CI) (CA INDEX NAME)



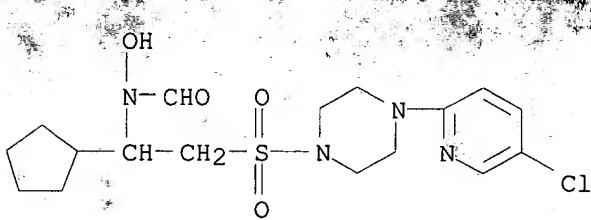
RN 260439-18-7 HCPLUS

CN Piperazine, 1-[(2-(formylhydroxyamino)-2-[4-(trifluoromethyl)phenyl]ethyl]sulfonyl-4-(2-pyridinyl)- (9CI) (CA INDEX NAME)

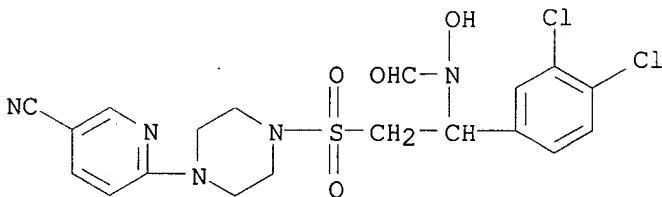


RN 260439-31-4 HCPLUS

CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[(2-cyclopentyl-2-(formylhydroxyamino)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

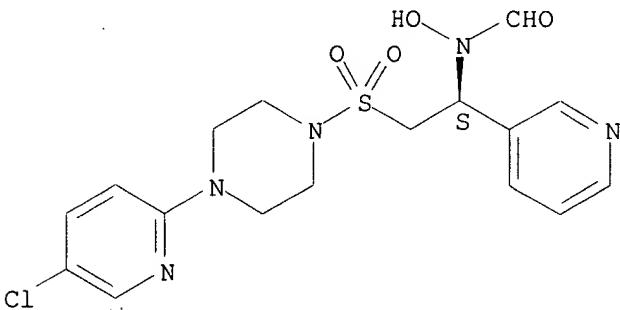


RN 260439-32-5 HCAPLUS  
 CN Piperazine, 1-(5-cyano-2-pyridinyl)-4-[[2-(3,4-dichlorophenyl)-2-(formylhydroxyamino)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

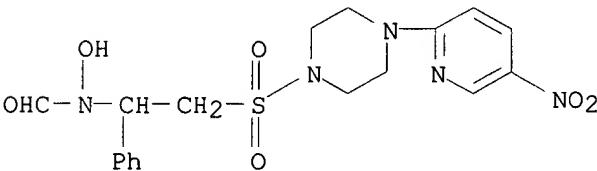


RN 260439-80-3 HCAPLUS  
 CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[(2S)-2-(formylhydroxyamino)-2-(3-pyridinyl)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

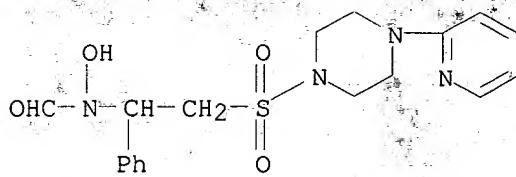
Absolute stereochemistry.



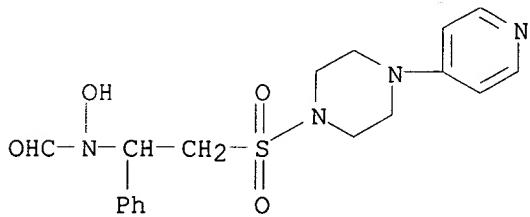
RN 260440-05-9 HCAPLUS  
 CN Piperazine, 1-[(2-(formylhydroxyamino)-2-phenylethyl)sulfonyl]-4-(5-nitro-2-pyridinyl)- (9CI) (CA INDEX NAME)



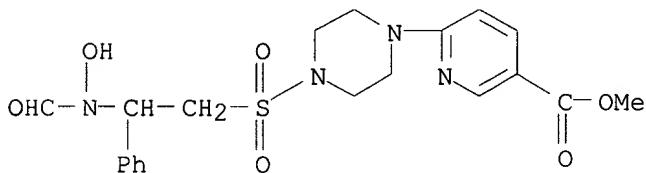
RN 260440-10-6 HCAPLUS  
 CN Piperazine, 1-[(2-(formylhydroxyamino)-2-phenylethyl)sulfonyl]-4-(2-pyridinyl)- (9CI) (CA INDEX NAME)



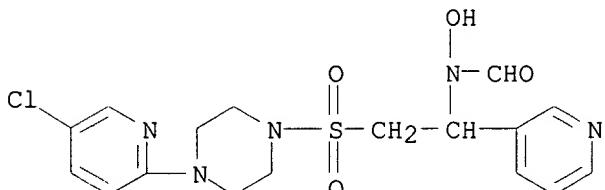
RN 260440-19-5 HCAPLUS  
 CN Piperazine, 1-[(2-(formylhydroxyamino)-2-phenylethyl)sulfonyl]-4-(4-pyridinyl)- (9CI) (CA INDEX NAME)



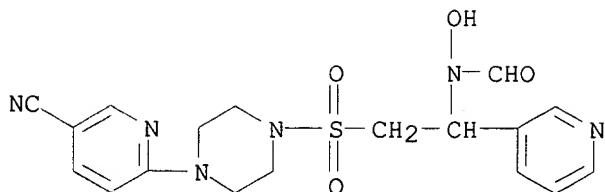
RN 260440-23-1 HCAPLUS  
 CN 3-Pyridinecarboxylic acid, 6-[4-[(2-(formylhydroxyamino)-2-phenylethyl)sulfonyl]piperazinyl]-, methyl ester (9CI) (CA INDEX NAME)



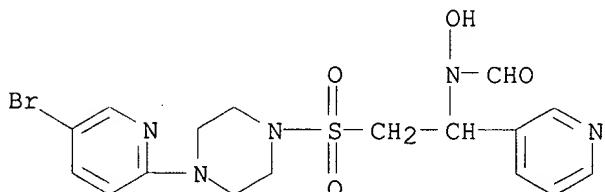
RN 260440-57-1 HCAPLUS  
 CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[(2-(formylhydroxyamino)-2-(3-pyridinyl)ethyl)sulfonyl]- (9CI) (CA INDEX NAME)



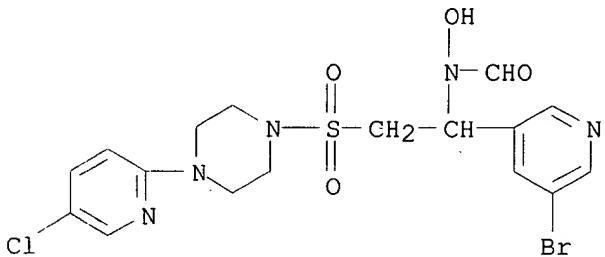
RN 260440-84-4 HCAPLUS  
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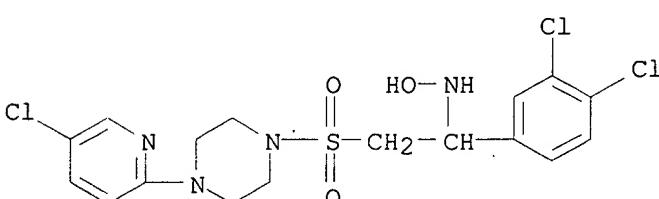
RN 260440-89-9 HCPLUS  
 CN Piperazine, 1-(5-bromo-2-pyridinyl)-4-[(2-(formylhydroxyamino)-2-(3-pyridinyl)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)



RN 260440-99-1 HCPLUS  
 CN Piperazine, 1-[(2-(5-bromo-3-pyridinyl)-2-(formylhydroxyamino)ethyl)sulfonyl]-4-(5-chloro-2-pyridinyl)- (9CI) (CA INDEX NAME)



IT 260441-75-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (prepn. of arylpiperazines as metalloproteinase inhibiting agents  
 (MMP))  
 RN 260441-75-6 HCPLUS  
 CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[(2-(3,4-dichlorophenyl)-2-(hydroxyamino)ethyl]sulfonyl]- (9CI) (CA INDEX NAME)

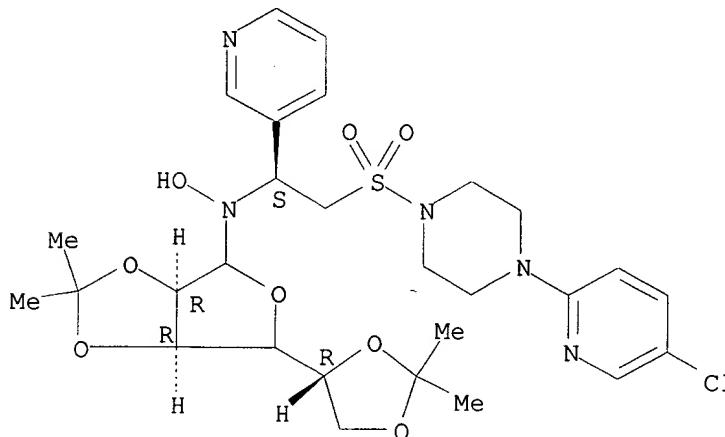


IT 260441-62-1P 260441-63-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. of arylpiperazines as metalloproteinase inhibiting agents  
 (MMP))

RN 260441-62-1 HCAPLUS

CN Piperazine, 1-[(2S)-2-[(4-oxo-2,3:5,6-bis-O-(1-methylethylidene)-D-ribohexofuranosyl]hydroxyamino]-2-(3-pyridinyl)ethylsulfonyl]-4-(5-chloro-2-pyridinyl)- (9CI) (CA INDEX NAME)

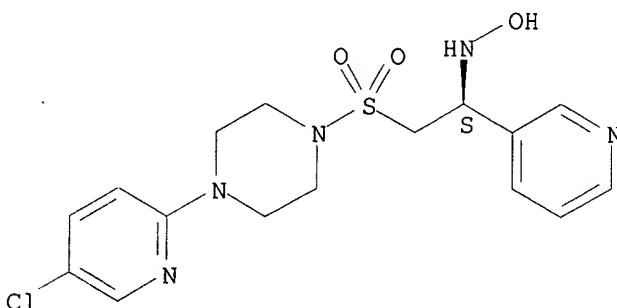
Absolute stereochemistry.



RN 260441-63-2 HCAPLUS

CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[(2S)-2-(hydroxyamino)-2-(3-pyridinyl)ethylsulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

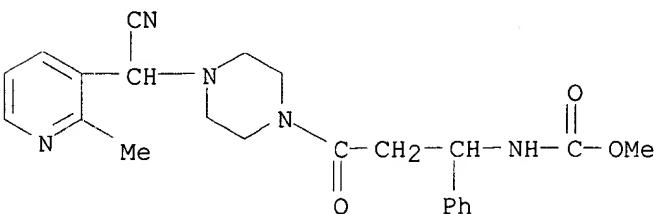
=> d ibib abs hitstr 116 4

L16 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1996:6879 HCAPLUS  
 DOCUMENT NUMBER: 124:176036  
 TITLE: Design, Synthesis, and Structure-Activity Relationship Studies of Novel 1-[(1-Acyl-4-piperidinyl)methyl]-1H-2-methylimidazo[4,5-c]pyridine Derivatives as Potent, Orally Active Platelet-Activating Factor Antagonists  
 AUTHOR(S): Carceller, Elena; Merlos, Manuel; Giral, Marta; Balsa, Dolors; Garcia-Rafanell, Julian; Forn, Javier  
 CORPORATE SOURCE: Research Center, J. Uriach Cia. S.A., Barcelona, 08026, Spain  
 SOURCE: Journal of Medicinal Chemistry (1996), 39(2), 487-93  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Replacement of the polar head of the previously reported series of 1-acyl-4-[(2-methyl-3-pyridyl)cyanomethyl]piperazines with a 2-methylimidazo[4,5-c]pyridine group led to the identification of a new series of 1-[(1-acyl-4-piperidinyl)methyl]-1H-2-methylimidazo[4,5-c]pyridine derivs. as potent, orally active platelet-activating factor (PAF) antagonists. On the basis of the general structure-activity relationship trends found for the acyl substituent in our earlier series, five groups of compds. were tested, i.e., diaryl- or alkylarylpropanoyl derivs., their 3-hydroxy-substituted analogs, and urea, carbamate and amino acid derivs. The optimal compd. UR-12670, bearing the 3,3-diphenylpropanoyl moiety, exhibited very high in vitro and in vivo potency ( $IC_{50} = 0.0076 \mu M$  for the in vitro PAF-induced platelet aggregation assay,  $ID_{50} = 0.0086 \text{ mg/kg}$  for the in vivo PAF-induced hypotension test in normotensive rats, and  $ID_{50} = 0.092 \text{ mg/kg po}$  and  $0.0008 \text{ mg/kg i.v.}$  for the PAF-induced mortality test in mice). UR-12670 also showed long duration of activity. It gave 100% protection against PAF-induced mortality in mice 7 h after i.v. administration of a single dose of 1 mg/kg and also provided 100% inhibition of PAF-induced aggregation in dog whole blood 6 h after i.v. administration of the same dose. The lead structure UR-12670 was selected for in-depth pharmacol. evaluation.

IT 149692-09-1  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
 (structure activity relationship of (piperidinyl)methylimidazo[4,5-c]pyridines as platelet activating factor antagonists)

RN 149692-09-1 HCAPLUS  
 CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-, methyl ester (9CI) (CA INDEX NAME)



=> d ibib abs hitstr 116 5

L16 ANSWER 5 OF 8 HCPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1995:380148 HCPLUS  
 DOCUMENT NUMBER: 122:160682  
 TITLE: Cyanomethylpyridine derivatives as PAF antagonists and  
       5-lipoxygenase inhibitors  
 INVENTOR(S): Carceller, Elena; Jimenez, Pere J.; Almansa, Carmen;  
               Bartoli, Javier  
 PATENT ASSIGNEE(S): J. Uriach y Cia. S.A., Spain  
 SOURCE: Eur. Pat. Appl., 25 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 617032	A1	19940928	EP 1994-104612	19940323
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
ES 2062943	A1	19941216	ES 1993-591	19930323
ES 2062943	B1	19951116		
CA 2118831	AA	19940924	CA 1994-2118831	19940311
JP 07002841	A2	19950106	JP 1994-76436	19940323
US 5420131	A	19950530	US 1994-216583	19940323
PRIORITY APPLN. INFO.:			ES 1993-591	19930323
OTHER SOURCE(S):	MARPAT	122:160682		
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

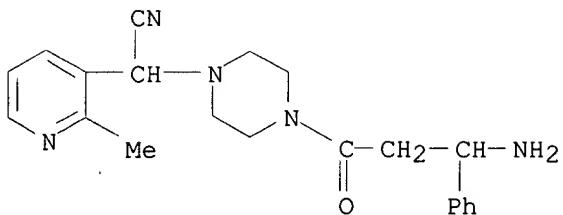
AB The invention relates to cyanomethylpyridine derivs. I [Y = N or CH; R1 = F, Cl; R2 = H or C1-4 alkyl; m = 0, 1 or 2; n = 0 or 1; p = 0 or 1; A = covalent bond, CONHCH(Ar), NHCH(Ar), SO2NHCH(Ar), NHCONHCH(Ar), or OCONHCH(Ar); and when p = 1, A can also = CH(Ar)NH; Ar = Ph or Ph substituted. gtoreq. 1 of halo, C1-4 alkyl, C1-4 alkoxy, or CF3]. The compds. are platelet activating factor (PAF) antagonists and/or 5-lipoxygenase inhibitors, and are useful for treating a variety of diseases. For example, coupling of p-(2-quinolylmethoxy)phenylacetic acid with 1-(3-amino-3-phenylpropionyl)-4-[2-methyl-3-pyridyl]cyanomethyl]piperazine using DCC and 1-hydroxybenzotriazole in DMF gave 43% title compd. II, a preferred compd. The IC50 of II for inhibition of PAF-induced hypotension in normotensive rats was 0.036 mg/kg i.v. Twelve addnl. syntheses, addnl. biol. tests (inhibition of PAF-induced platelet aggregation, and inhibition of LTB4 prodn.), and 6 example formulations are given.

IT 149691-83-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (amidation; prepn. of cyanomethylpyridine derivs. as PAF antagonists  
 and 5-lipoxygenase inhibitors)

RN 149691-83-8 HCPLUS

CN 1-Piperazineacetonitrile, 4-(3-amino-1-oxo-3-phenylpropyl)-.alpha.- (2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)



IT 161180-94-5P 161180-95-6P 161180-96-7P

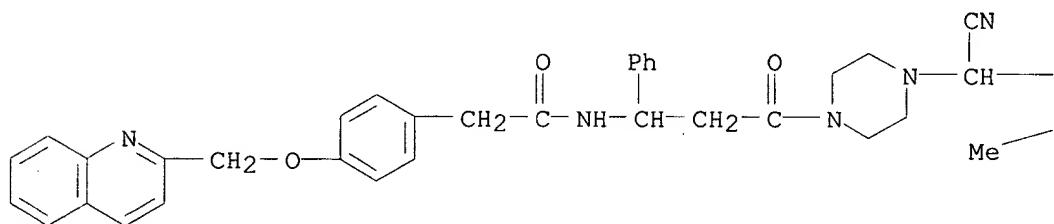
161180-97-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of cyanomethylpyridine derivs. as PAF antagonists and 5-lipoxygenase inhibitors)

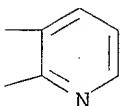
RN 161180-94-5 HCPLUS

CN Benzeneacetamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-3-(2-quinolinylmethoxy)- (9CI) (CA INDEX NAME)

PAGE 1-A



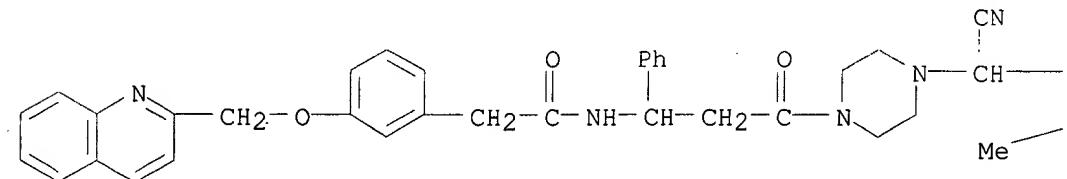
PAGE 1-B

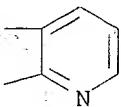


RN 161180-95-6 HCPLUS

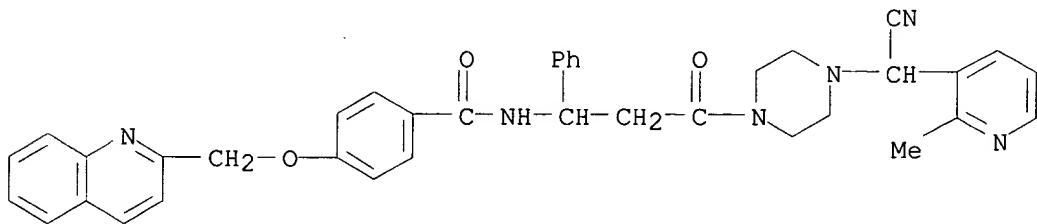
CN Benzeneacetamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-3-(2-quinolinylmethoxy)- (9CI) (CA INDEX NAME)

PAGE 1-A

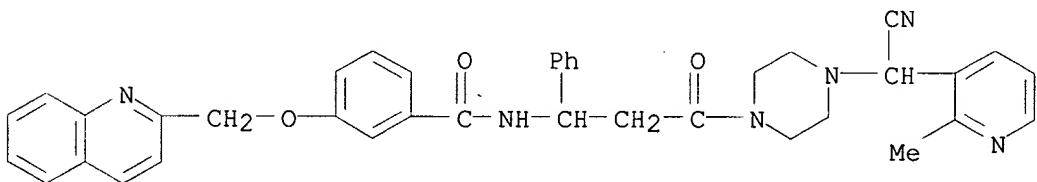




RN 161180-96-7 HCAPLUS  
 CN Benzamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-4-(2-quinolinylmethoxy)- (9CI) (CA INDEX NAME)

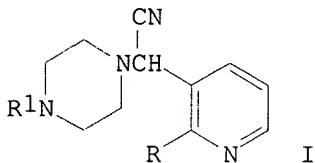


RN 161180-97-8 HCAPLUS  
 CN Benzamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-3-(2-quinolinylmethoxy)- (9CI) (CA INDEX NAME)



=> d ibib abs hitstr 116 6

L16 ANSWER 6 OF 8 HCPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1994:106931 HCPLUS  
 DOCUMENT NUMBER: 120:106931  
 TITLE: Synthesis and structure-activity relationships of  
 1-acyl-4-((2-methyl-3-pyridyl)cyanomethyl)piperazines  
 as PAF antagonists  
 AUTHOR(S): Carceller, Elena; Merlos, Manuel; Giral, Marta;  
 Almansa, Carmen; Bartroli, Javier; Garcia-Rafanell,  
 Julian; Forn, Javier  
 CORPORATE SOURCE: Chem. Lab., J. Uriach e Cia.S.A., Barcelona, 08026,  
 Spain  
 SOURCE: Journal of Medicinal Chemistry (1993), 36(20), 2984-97  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



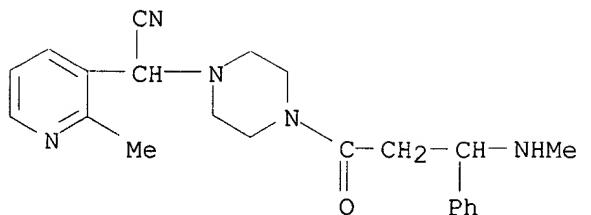
AB Title compds., e.g. I [R = Me, R1 = Ph<sub>2</sub>CHXCH<sub>2</sub>CO, PhCR<sub>2</sub>R<sub>3</sub>CH<sub>2</sub>CO, R<sub>4</sub>NHCHPhCO; X = CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>, NH, NCHO, NAc, NSO<sub>2</sub>Me, O, S(O), SO<sub>2</sub>; R<sub>2</sub> = OH, CO<sub>2</sub>Et, F, R<sub>3</sub> = Ph, Me, CF<sub>3</sub>, 3-pyridyl; R<sub>4</sub> = PhO<sub>2</sub>C, PhCH<sub>2</sub>O<sub>2</sub>C, MeO<sub>2</sub>C, EtO<sub>2</sub>C, Me<sub>2</sub>CHCH<sub>2</sub>O<sub>2</sub>C, Me<sub>3</sub>CO<sub>2</sub>C, H<sub>2</sub>NCO, pyrrolidinocarbonyl, Bz, 3-pyridylcarbonyl, 3-furylcarbonyl, 2-piperazinylcarbonyl, Ac, Me, PhSO<sub>2</sub>, MeSO<sub>2</sub>, H, Ph, PhCH<sub>2</sub>, 3-pyridylmethyl, H<sub>2</sub>C:CHCH<sub>2</sub>, HC.tplbond.CCH<sub>2</sub>], second generation (cyanomethyl)piperazines with increased oral activity were prepd. and evaluated in vitro in a platelet aggregation factor (PAF)-induced platelet aggregation assay and in vivo in a PAF-induced hypotension test in normotensive rats. Oral activity was ascertained through a PAF-induced mortality test in mice. I (R = Me) showed an order of magnitude or greater improvement in the oral ID<sub>50</sub> test compared with I (R = H). Three different types of acyl substituents of similar potency emerge from this work: R<sub>1</sub> = Ph<sub>2</sub>CHNHCH<sub>2</sub>CO, HOCR<sub>3</sub>PhCH<sub>2</sub>CO, and R<sub>4</sub>NHCHPhCH<sub>2</sub>CO. The most interesting compds., I (R = Me, R<sub>1</sub> = Ph<sub>2</sub>CHNHCH<sub>2</sub>CO) (II) (UR-12460) and I (R = Me, R<sub>1</sub> = MeO<sub>2</sub>CNHCHPhCH<sub>2</sub>CO) (UR-12519) (III) compare favorably with WEB-2086. II and III were also tested in active anaphylactic shock and endotoxin-induced mortality tests. On the basis of these data and addnl. pharmacol. development, II and III were selected for clin. testing.

IT 149692-22-8 149692-25-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (platelet aggregation factor antagonistic activity of)

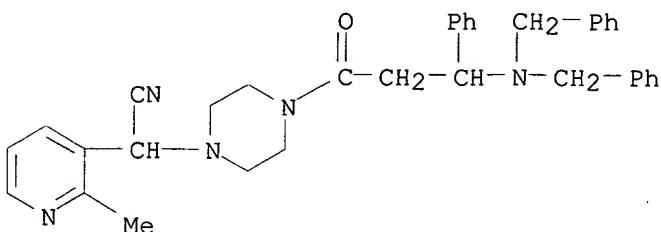
RN 149692-22-8 HCPLUS

CN 1-Piperazineacetonitrile, 4-[3-(methylamino)-1-oxo-3-phenylpropyl]-.alpha.-  
 (2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 149692-25-1 HCPLUS

CN 1-Piperazineacetonitrile, 4-[3-[bis(phenylmethyl)amino]-1-oxo-3-phenylpropyl]-.alpha.-(2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)

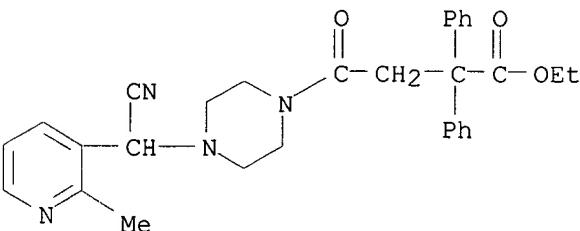
IT 149691-77-0P 149691-84-9P 149691-85-0P  
149691-86-1P 149692-10-4P 149692-11-5P  
149692-12-6P 149692-13-7P 149692-14-8P  
149692-15-9P 149692-16-0P 149692-17-1P  
149692-18-2P 149692-20-6P 149692-21-7P  
149692-24-0P 149692-26-2P 149692-27-3P  
149692-28-4P 149692-29-5P 149692-30-8P  
149692-31-9P 149692-41-1P 150812-47-8P  
150812-48-9P 150812-49-0P 150812-50-3P  
150812-51-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and platelet aggregation factor antagonistic activity of)

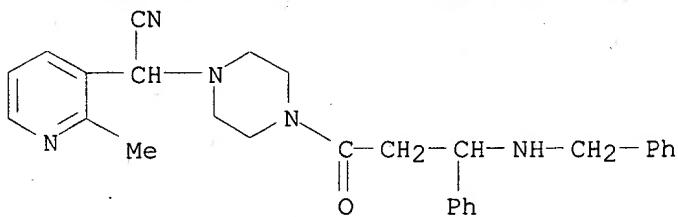
RN 149691-77-0 HCPLUS

CN 1-Piperazinebutanoic acid, 4-[cyano(2-methyl-3-pyridinyl)methyl]-.gamma.-oxo-.alpha.,.alpha.-diphenyl-, ethyl ester (9CI) (CA INDEX NAME)



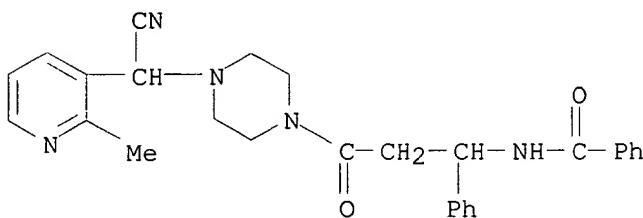
RN 149691-84-9 HCPLUS

CN 1-Piperazineacetonitrile, .alpha.-(2-methyl-3-pyridinyl)-4-[1-oxo-3-phenyl-3-[ (phenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)



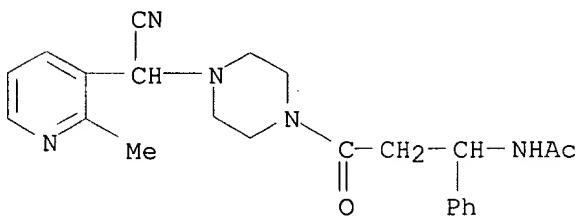
RN 149691-85-0 HCPLUS

CN Benzamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]- (9CI) (CA INDEX NAME)



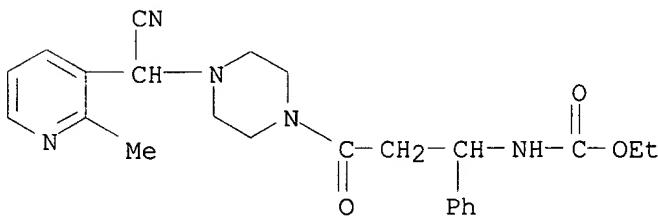
RN 149691-86-1 HCPLUS

CN Acetamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]- (9CI) (CA INDEX NAME)



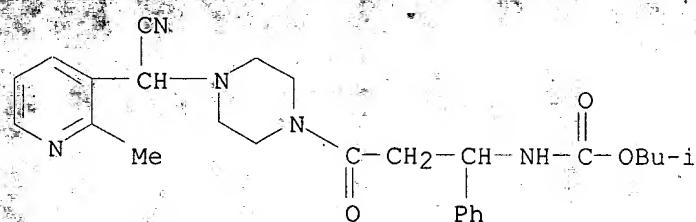
RN 149692-10-4 HCPLUS

CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-, ethyl ester (9CI) (CA INDEX NAME)



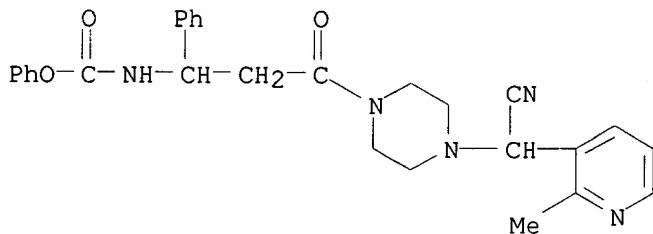
RN 149692-11-5 HCPLUS

CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)



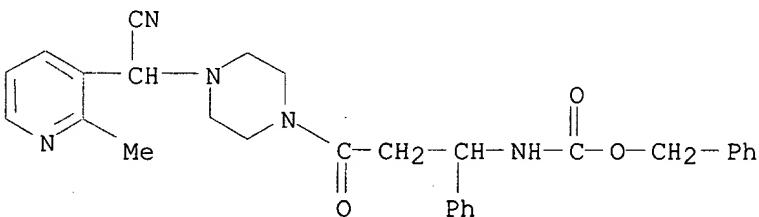
RN 149692-12-6 HCAPLUS

CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-, phenyl ester (9CI) (CA INDEX NAME)



RN 149692-13-7 HCAPLUS

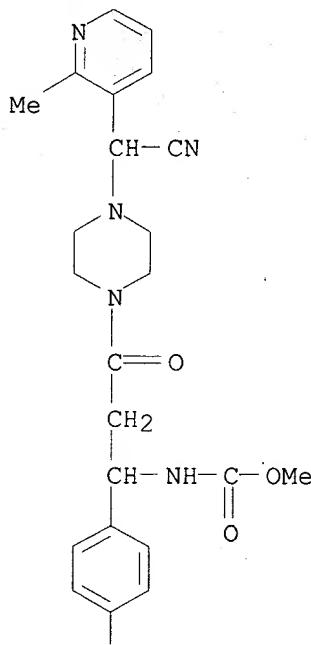
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RN 149692-14-8 HCAPLUS

CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-[4-(trifluoromethyl)phenyl]propyl]-, methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

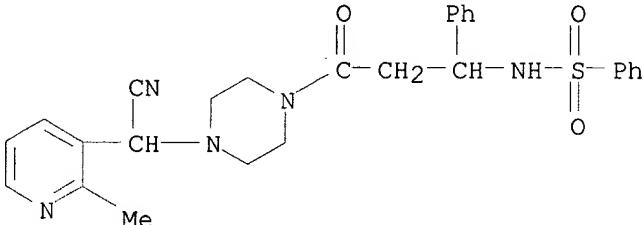


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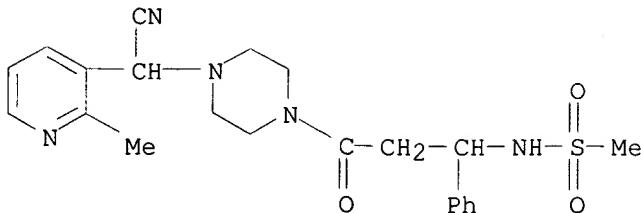
RN 149692-15-9 HCPLUS

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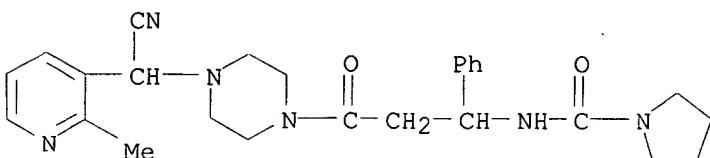
RN 149692-16-0 HCPLUS

CN 1-Piperazineacetonitrile, .alpha.- (2-methyl-3-pyridinyl)-4-[3-[(methylsulfonyl)amino]-1-oxo-3-phenylpropyl]- (9CI) (CA INDEX NAME)



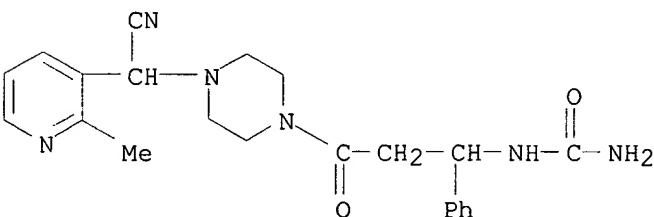
RN 149692-17-1 HCAPLUS

CN 1-Pyrrolidinecarboxamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]- (9CI) (CA INDEX NAME)



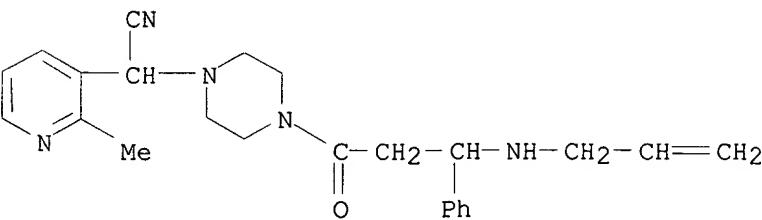
RN 149692-18-2 HCAPLUS

CN 1-Piperazineacetonitrile, 4-[3-[(aminocarbonyl)amino]-1-oxo-3-phenylpropyl]-.alpha.- (2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 149692-20-6 HCAPLUS

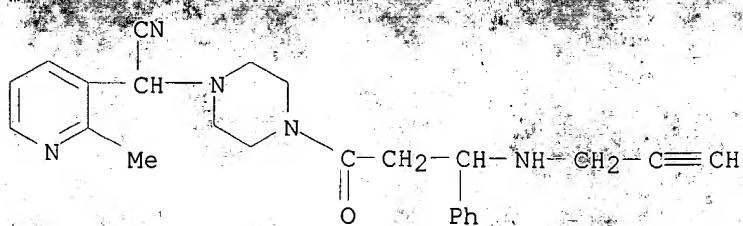
CN 1-Piperazineacetonitrile, .alpha.- (2-methyl-3-pyridinyl)-4-[1-oxo-3-phenyl-3-(2-propenylamino)propyl]-, trihydrochloride (9CI) (CA INDEX NAME)



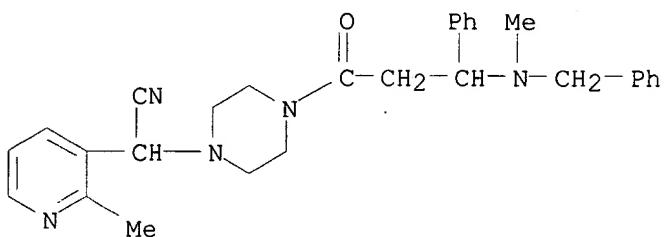
● 3 HCl

RN 149692-21-7 HCAPLUS

CN 1-Piperazineacetonitrile, .alpha.- (2-methyl-3-pyridinyl)-4-[1-oxo-3-phenyl-3-(2-propenylamino)propyl]- (9CI) (CA INDEX NAME)

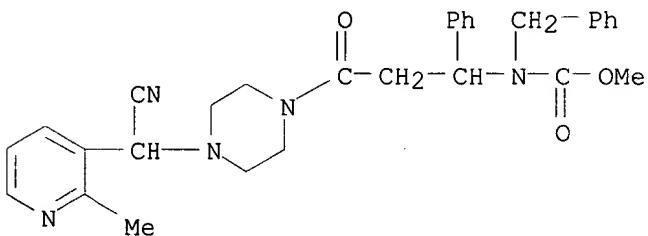


RN 149692-24-0 HCAPLUS  
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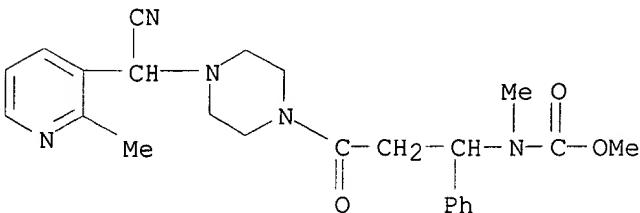


● 2 HCl

RN 149692-26-2 HCAPLUS  
 CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl](phenylmethyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 149692-27-3 HCAPLUS  
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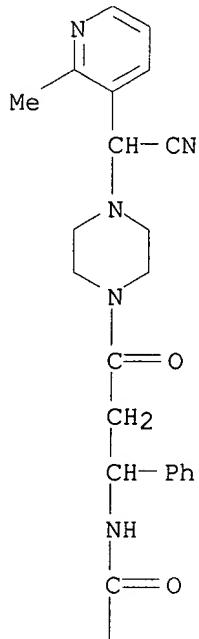


RN 149692-28-4 HCAPLUS  
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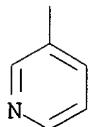
Habte 09\_980593

piperazinyl]-3-oxo-1-phenylpropyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



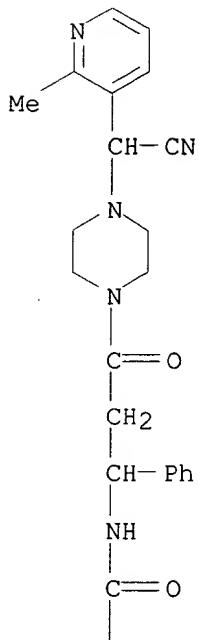
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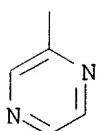
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CN Pyrazinecarboxamide, N-[3-{4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl}-3-oxo-1-phenylpropyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

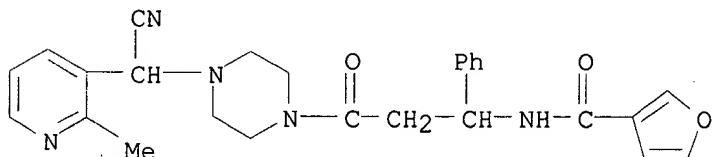


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RN 149692-30-8 HCPLUS

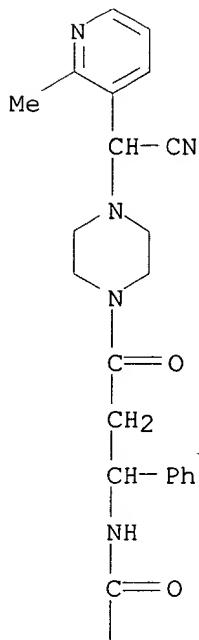
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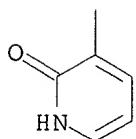
RN 149692-31-9 HCPLUS

CN 3-Pyridinecarboxamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-1,2-dihydro-2-oxo- (9CI) (CA INDEX NAME)

PAGE 1-A

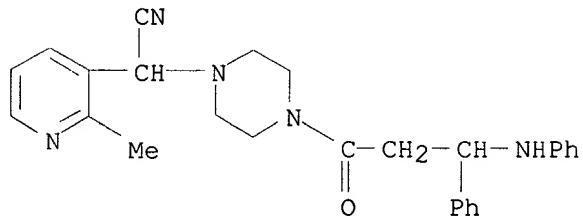


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RN 149692-41-1 HCAPLUS

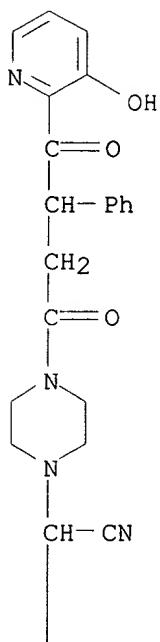
CN 1-Piperazineacetonitrile, .alpha.-{(2-methyl-3-pyridinyl)-4-[1-oxo-3-phenyl-3-(phenylamino)propyl]}- (9CI) (CA INDEX NAME)



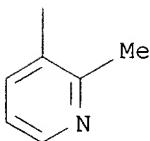
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CN 1-Piperazineacetonitrile, 4-[4-(3-hydroxy-2-pyridinyl)-1,4-dioxo-3-phenylbutyl]-.alpha.-{(2-methyl-3-pyridinyl)}- (9CI) (CA INDEX NAME)

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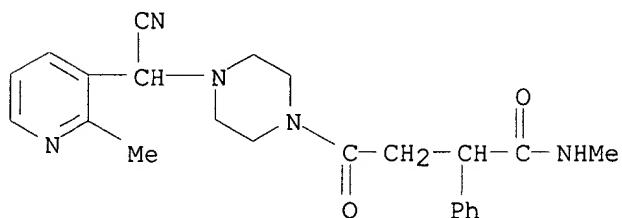


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RN 150812-48-9 HCAPLUS

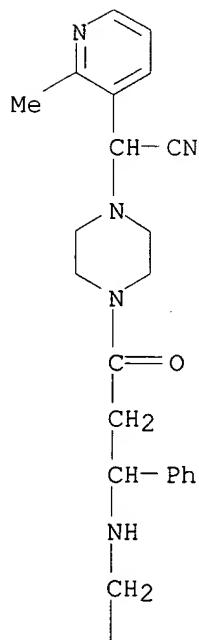
CN 1-Piperazinebutanamide, 4-[cyano(2-methyl-3-pyridinyl)methyl]-N-methyl-.gamma.-oxo-.alpha.-phenyl- (9CI) (CA INDEX NAME)



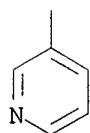
RN 150812-49-0 HCAPLUS

CN 1-Piperazineacetonitrile, .alpha.-.(2-methyl-3-pyridinyl)-4-[1-oxo-3-phenyl-3-[(3-pyridinylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)

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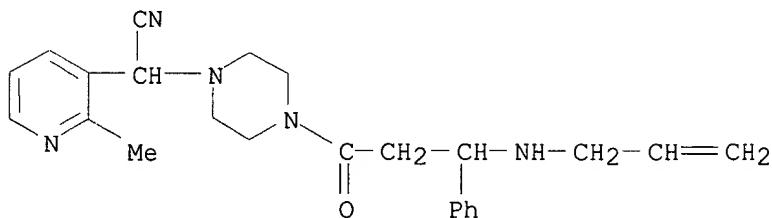


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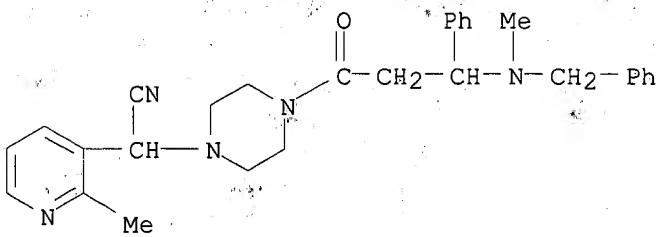
RN 150812-50-3 HCAPLUS

CN 1-Piperazineacetonitrile, .alpha.- (2-methyl-3-pyridinyl)-4-[1-oxo-3-phenyl-3-(2-propenylamino)propyl]- (9CI) (CA INDEX NAME)



RN 150812-51-4 HCAPLUS

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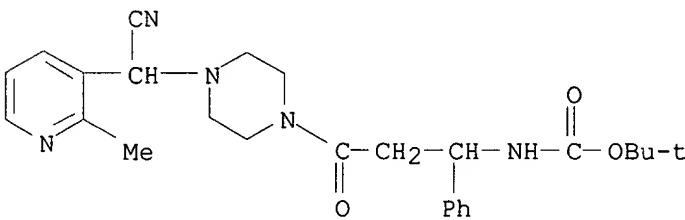


IT 149691-82-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn., deprotection, and platelet aggregation factor antagonistic activity of)

RN 149691-82-7 HCPLUS

CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

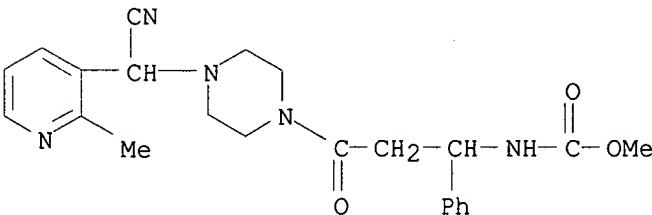


IT 149692-09-1P, UR 12519

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn., platelet aggregation factor antagonistic activity, and toxicity of)

RN 149692-09-1 HCPLUS

CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-, methyl ester (9CI) (CA INDEX NAME)



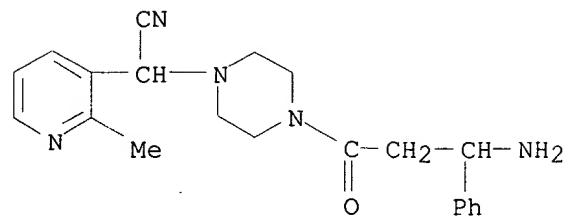
IT 149691-83-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn., reactions, and platelet aggregation factor antagonistic activity of)

RN 149691-83-8 HCPLUS

CN 1-Piperazineacetonitrile, 4-(3-amino-1-oxo-3-phenylpropyl)-.alpha.- (2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE COVERS 1907-1966  
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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L17 O L15

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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STRUCTURE FILE UPDATES: 19 MAR 2003 HIGHEST RN 500101-42-8  
DICTIONARY FILE UPDATES: 19 MAR 2003 HIGHEST RN 500101-42-8

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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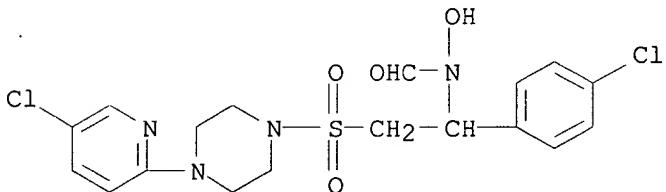
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L15 ANSWER 1 OF 80 REGISTRY COPYRIGHT 2003 ACS  
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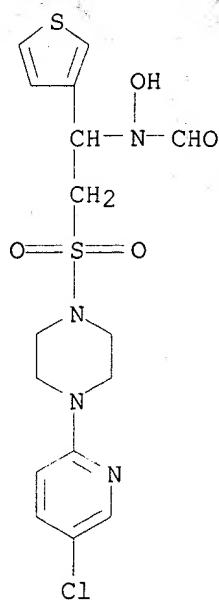


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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 135:211053

L15 ANSWER 2 OF 80 REGISTRY COPYRIGHT 2003 ACS  
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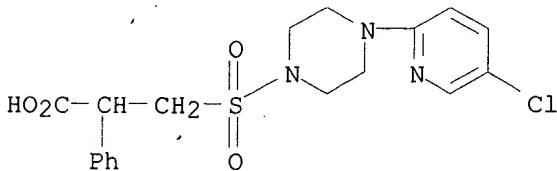


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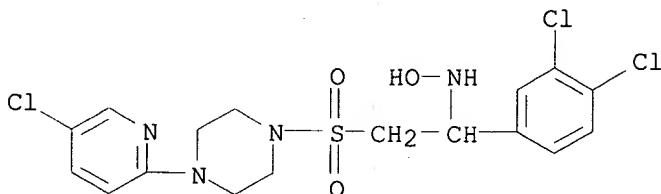
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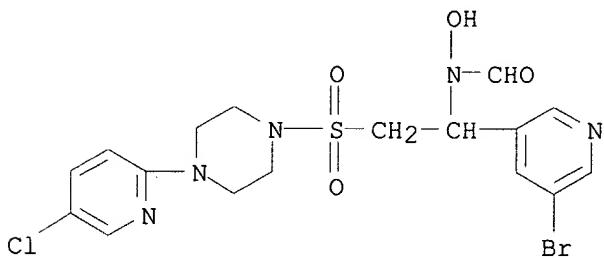


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REFERENCE 1: 132:207849

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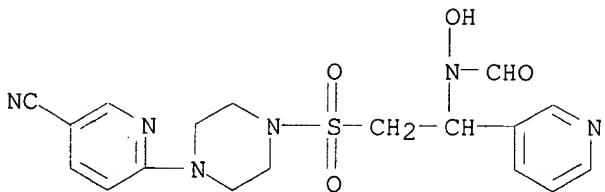


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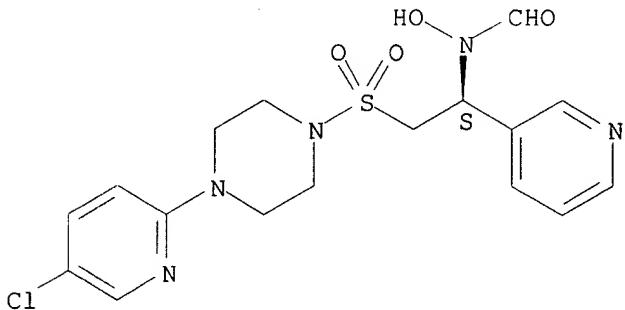
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Absolute stereochemistry.

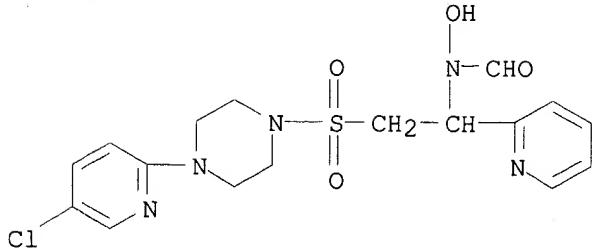


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REFERENCE 1: 132:207849

L15 ANSWER 29 OF 80 REGISTRY COPYRIGHT 2003 ACS  
RN 260438-37-7 REGISTRY  
CN Piperazine, 1-(5-chloro-2-pyridinyl)-4-[(2S)-2-(formylhydroxyamino)-2-(3-pyridinyl)ethylsulfonyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C17 H20 Cl N5 O4 S  
SR CA  
LC STN Files: CA, CAPLUS

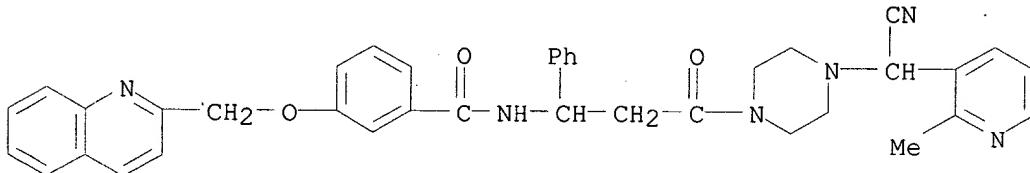


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 132:207849

L15 ANSWER 33 OF 80 REGISTRY COPYRIGHT 2003 ACS  
 RN 161180-97-8 REGISTRY  
 CN Benzamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-3-(2-quinolinylmethoxy)- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C38 H36 N6 O3  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

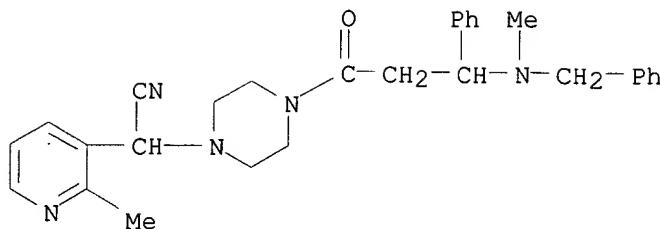


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 122:160682

L15 ANSWER 37 OF 80 REGISTRY COPYRIGHT 2003 ACS  
 RN 150812-51-4 REGISTRY  
 CN 1-Piperazineacetonitrile, 4-[3-[methyl(phenylmethyl)amino]-1-oxo-3-phenylpropyl]-.alpha.- (2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C29 H33 N5 O  
 CI COM  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

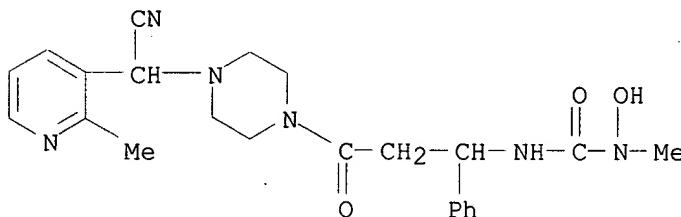


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 120:106931

L15 ANSWER 42 OF 80 REGISTRY COPYRIGHT 2003 ACS  
RN 149692-45-5 REGISTRY  
CN 1-Piperazineacetonitrile, 4-[3-[(hydroxymethylamino)carbonyl]amino]-1-oxo-3-phenylpropyl-α-(2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C23 H28 N6 O3  
SR CA  
LC STN Files: CA, CAPLUS

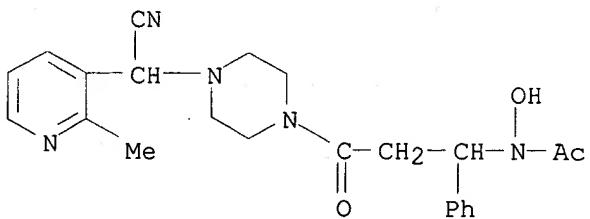


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 119:139266

L15 ANSWER 45 OF 80 REGISTRY COPYRIGHT 2003 ACS  
RN 149692-42-2 REGISTRY  
CN Acetamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]-N-hydroxy- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C23 H27 N5 O3  
SR CA  
LC STN Files: CA, CAPLUS

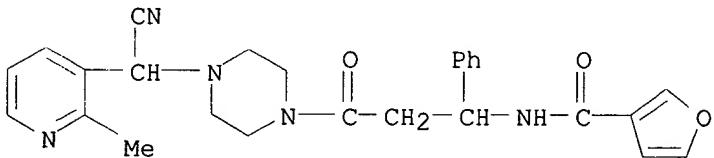


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 119:139266

L15 ANSWER 50 OF 80 REGISTRY COPYRIGHT 2003 ACS  
 RN 149692-30-8 REGISTRY  
 CN 3-Furancarboxamide, N-[3-[4-[(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C26 H27 N5 O3  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER



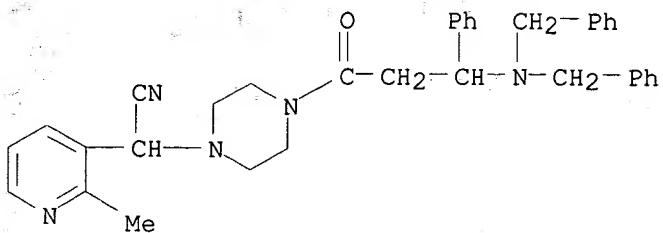
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1962 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 120:106931

REFERENCE 2: 119:139266

L15 ANSWER 55 OF 80 REGISTRY COPYRIGHT 2003 ACS  
 RN 149692-25-1 REGISTRY  
 CN 1-Piperazineacetonitrile, 4-[(3-[(2S)-2-[(2S)-2-((2S)-2-methyl-3-pyridinyl)ethyl]amino]-3-oxo-3-phenylpropyl)-.alpha.- (2-methyl-3-pyridinyl)- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C35 H37 N5 O  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

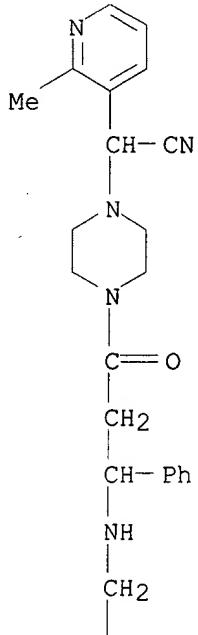
2 REFERENCES IN FILE CA (1962 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 120:106931

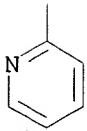
REFERENCE 2: 119:139266

L15 ANSWER 60 OF 80 REGISTRY COPYRIGHT 2003 ACS  
 RN 149692-19-3 REGISTRY  
 CN 1-Piperazineacetonitrile, .alpha.-.(2-methyl-3-pyridinyl)-4-[1-oxo-3-phenyl-  
 3-[(2-pyridinylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C27 H30 N6 O  
 SR CA  
 LC STN Files: CA, CAPLUS

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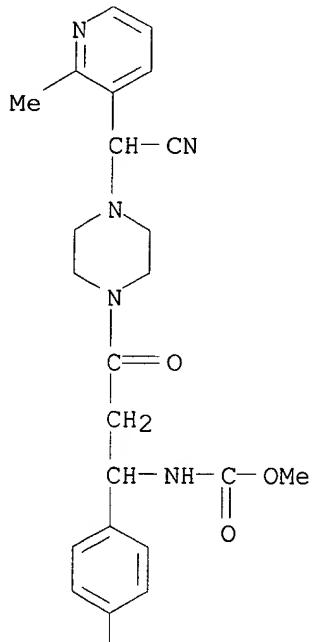
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 119:139266

L15 ANSWER 65 OF 80 REGISTRY COPYRIGHT 2003 ACS  
 RN 149692-14-8 REGISTRY  
 CN Carbamic acid, [3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-[4-(trifluoromethyl)phenyl]propyl-, methyl ester (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C24 H26 F3 N5 O3  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

PAGE 1-A



PAGE 2-A



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1962 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 120:106931

REFERENCE 2: 119:139266

L15 ANSWER 71 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 149691-86-1 REGISTRY

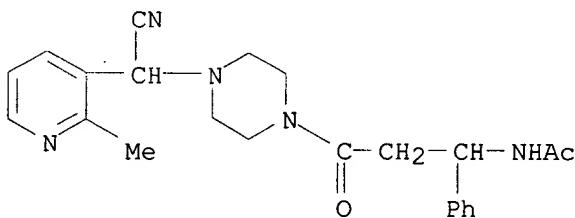
CN Acetamide, N-[3-[4-[cyano(2-methyl-3-pyridinyl)methyl]-1-piperazinyl]-3-oxo-1-phenylpropyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C23 H27 N5 O2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1962 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 120:106931

REFERENCE 2: 119:139266

L15 ANSWER 77 OF 80 REGISTRY COPYRIGHT 2003 ACS

RN 121118-99-8 REGISTRY

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[[4-[(4,5-dihydroxy-2-pyridinyl)methyl]-2,3-dioxo-1-piperazinyl]carbonyl]amino]phenylacetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, monosodium salt, [2S-[2.alpha.,5.alpha.,6.beta.(S\*)]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

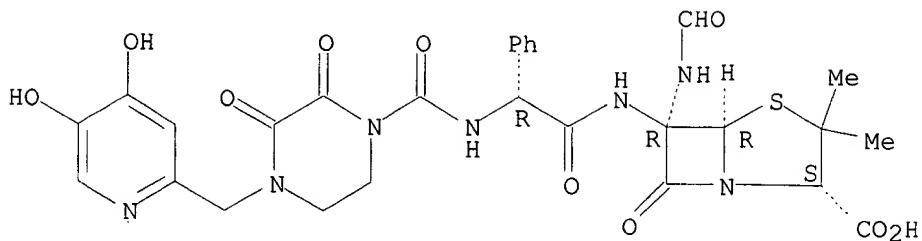
MF C28 H29 N7 O10 S . Na

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

CRN (121102-21-4)

Absolute stereochemistry.



● Na

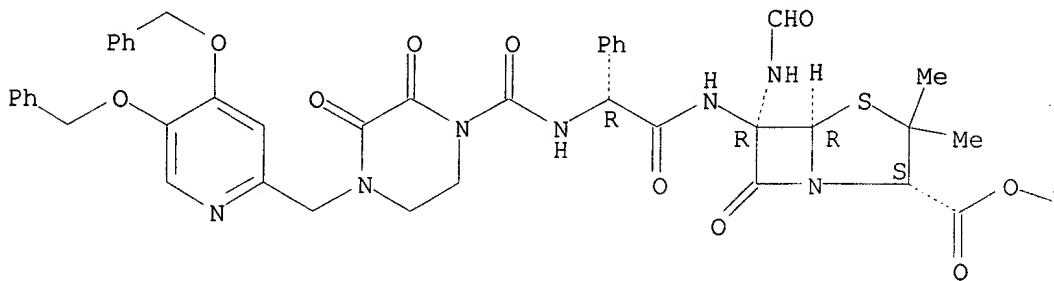
1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 111:39092

L15 ANSWER 78 OF 80 REGISTRY COPYRIGHT 2003 ACS  
 RN 121102-36-1 REGISTRY  
 CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[[4-[4,5-bis(phenylmethoxy)-2-pyridinyl]methyl]-2,3-dioxo-1-piperazinyl]carbonyl]amino]phenylacetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, phenylmethyl ester, [2S-[2.alpha.,5.alpha.,6.beta.(S\*)]]-(9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C49 H47 N7 O10 S  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

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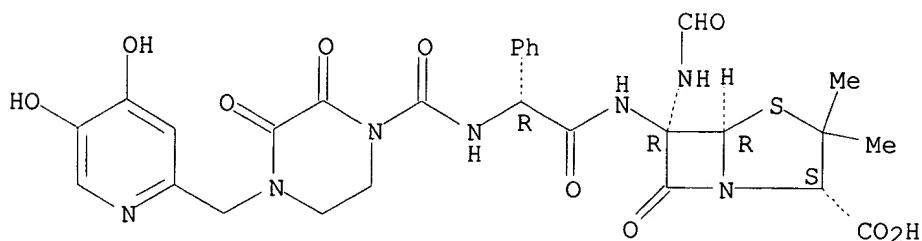
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 111:39092

L15 ANSWER 80 OF 80 REGISTRY COPYRIGHT 2003 ACS  
 RN 121102-21-4 REGISTRY  
 CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[4-[(4,5-dihydroxy-2-pyridinyl)methyl]-2,3-dioxo-1-piperazinyl]carbonyl]amino]phenylacetyl]amino]-6-(formylamino)-3,3-dimethyl-7-oxo-, [2S-[2.alpha.,5.alpha.,6.beta.-(S\*)]]- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C28 H29 N7 O10 S  
 CI COM  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 111:39092